

Butyl butyrate
109-21-7 | DTXSID7041702

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.99e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.23e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

Image not found

Butyl butyrate

Measured: 3.47e-03

Predicted: 6.99e-03

Image not found

Pentyl propionate

Measured: 5.62e-03

Predicted: 7.41e-03

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Acetic acid, 2-ethylbutyl ester

Measured: 4.44e-02

Predicted: 1.03e-02

Image not found

Ethyl hexanoate

Measured: 4.36e-03

Predicted: 6.07e-03

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1,3-Dimethylbutyl acetate

Measured: 9.01e-03

Predicted: 8.99e-03